

INTEGRAL FORM OF THE SCHRÖDINGER EQUATION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 11.8.

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As a prelude to the Born approximation in quantum scattering, we need to look at the integral form of the time-independent Schrödinger equation. The equation in its original differential equation form is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad (1)$$

which can be written as

$$(\nabla^2 + k^2)\psi = Q \quad (2)$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad (3)$$

$$Q \equiv \frac{2m}{\hbar^2}V\psi \quad (4)$$

To convert this to an integral equation, we need to define a *Green's function* $G(\mathbf{r})$ which satisfies the differential equation

$$(\nabla^2 + k^2)G(\mathbf{r}) = \delta^3(\mathbf{r}) \quad (5)$$

Using this function we can write ψ as an integral equation

$$\psi(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}_0)Q(\mathbf{r}_0)d^3\mathbf{r}_0 \quad (6)$$

We can show this works by plugging in G from 5:

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = \int (\nabla^2 + k^2)G(\mathbf{r} - \mathbf{r}_0)Q(\mathbf{r}_0)d^3\mathbf{r}_0 \quad (7)$$

$$= \int \delta(\mathbf{r} - \mathbf{r}_0)Q(\mathbf{r}_0)d^3\mathbf{r}_0 \quad (8)$$

$$= Q(\mathbf{r}) \quad (9)$$

which gives us back 2.

This isn't a solution of the Schrödinger equation, of course, because Q contains ψ , so we'd need to actually know ψ in advance in order to work out the integral with the Green's function. Rather, it's just a different way of writing the Schrödinger equation which proves useful in scattering theory.

Because 5 doesn't depend on the potential V , we can work out the Green's function which is valid for every potential. The process is rather involved, but Griffiths goes through the details in section 11.4.1, so I won't reproduce them here, apart from noting that the solution uses what is, to me, one of the most beautiful theorems in mathematics: Cauchy's theorem on contour integration. Maybe I'll return to it later.

Anyway, the Green's function turns out to be

$$G(\mathbf{r}) = -\frac{e^{ikr}}{4\pi r} \quad (10)$$

We can verify this is in fact a solution by plugging it back into 5. We need the Laplacian of G which we can get by calculating the divergence of the gradient. Taking the gradient first, we use the product rule for gradients:

$$\nabla(fg) = f\nabla g + g\nabla f \quad (11)$$

We get

$$\nabla G = -\frac{1}{4\pi} \left(\frac{1}{r} \nabla e^{ikr} + e^{ikr} \nabla \frac{1}{r} \right) \quad (12)$$

To calculate the divergence of the gradient, we use the identity for the divergence of the product of a scalar and a vector:

$$\nabla \cdot (f\mathbf{A}) = \mathbf{A} \cdot \nabla f + f\nabla \cdot \mathbf{A} \quad (13)$$

We therefore have

$$\nabla^2 G = -\frac{1}{4\pi} \left[\left(\nabla \frac{1}{r} \right) \cdot \left(\nabla e^{ikr} \right) + \frac{1}{r} \nabla^2 e^{ikr} + \left(\nabla e^{ikr} \right) \cdot \left(\nabla \frac{1}{r} \right) + e^{ikr} \nabla^2 \left(\frac{1}{r} \right) \right]$$

The last term turns out to be a delta function:

$$\nabla^2 \frac{1}{r} = \nabla \cdot \left(\nabla \frac{1}{r} \right) = -\nabla \cdot \left(\frac{\hat{\mathbf{r}}}{r^2} \right) = -4\pi \delta^3(\mathbf{r}) \quad (15)$$

To work out the second term, we use the formula for the Laplacian in spherical coordinates, for a function that depends only on r :

$$\nabla^2 f(r) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) \quad (16)$$

We get

$$\nabla^2 e^{ikr} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(ikr^2 e^{ikr} \right) \quad (17)$$

$$= \frac{2ik}{r} e^{ikr} - k^2 e^{ikr} \quad (18)$$

Putting this back into 14 we get

$$\nabla^2 G = -\frac{1}{4\pi} \left[2 \left(\nabla \frac{1}{r} \right) \cdot \left(\nabla e^{ikr} \right) + \frac{2ik}{r^2} e^{ikr} - \frac{k^2}{r} e^{ikr} - 4\pi \delta^3(\mathbf{r}) e^{ikr} \right] \quad (19)$$

$$= -\frac{1}{4\pi} \left[-\frac{2ik}{r^2} e^{ikr} + \frac{2ik}{r^2} e^{ikr} - \frac{k^2}{r} e^{ikr} - 4\pi \delta^3(\mathbf{r}) e^{ikr} \right] \quad (20)$$

$$= -\frac{1}{4\pi} \left[-\frac{k^2}{r} e^{ikr} - 4\pi \delta^3(\mathbf{r}) \right] \quad (21)$$

$$= \frac{k^2}{4\pi r} e^{ikr} + \delta^3(\mathbf{r}) \quad (22)$$

$$= -k^2 G(\mathbf{r}) + \delta^3(\mathbf{r}) \quad (23)$$

$$(\nabla^2 + k^2) G(\mathbf{r}) = \delta^3(\mathbf{r}) \quad (24)$$

where we dropped the e^{ikr} from the last term in the third line since the delta function is zero except when $\mathbf{r} = 0$.

Using this Green's function, the integral form of the Schrödinger equation is

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} V(\mathbf{r}_0) \psi(\mathbf{r}_0) d^3\mathbf{r}_0 \quad (25)$$

where ψ_0 is a solution of the free particle Schrödinger equation

$$(\nabla^2 + k^2) \psi_0(\mathbf{r}) = 0 \quad (26)$$

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